

Neopentyl trimethylsilyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, neopentyl trimethylsilyl ester
Inchi:	InChI=1S/C16H24O4Si/c1-16(2,3)11-19-14(17)12-9-7-8-10-13(12)15(18)20-21(4,5)6/h7-
InchiKey:	RVDZCIVUEIELJN-UHFFFAOYSA-N
Formula:	C16H24O4Si
SMILES:	CC(C)(C)COC(=O)c1ccccc1C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	308.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.28		Crippen Method
logp	3.881		Crippen Method
rinpol	1815.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373491&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/19-664-4/Neopentyl-trimethylsilyl-phthalate.pdf>

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